



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:59 PM UTC

PDB ID : 4BY6 / pdb_00004by6
Title : Yeast Not1-Not2-Not5 complex
Authors : Bhaskar, V.; Basquin, J.; Conti, E.
Deposited on : 2013-07-18
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

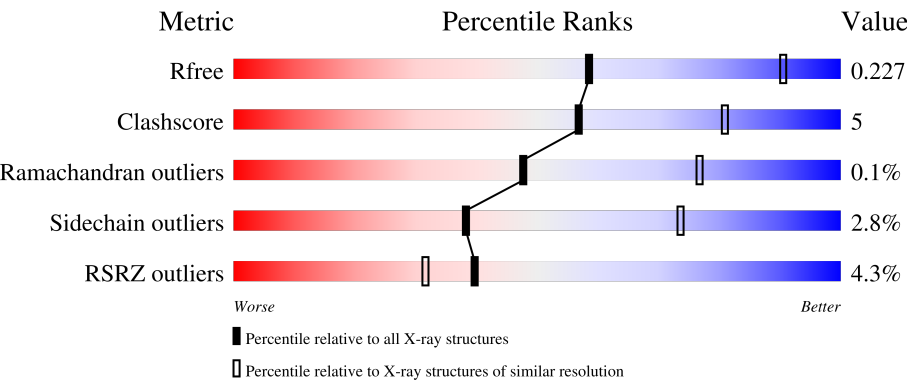
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	553	3% 79% 11% • 8%
1	D	553	4% 79% 12% 9%
2	B	191	4% 71% 15% • 13%
2	E	191	5% 74% 13% • 12%
3	C	262	4% 61% 6% 33%

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Mol	Chain	Length	Quality of chain
3	F	262	4% 61% 6% 33%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14028 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			4141	2721	666	743	11			
1	D	504	Total	C	N	O	S	0	0	0
			4116	2707	659	739	11			

- Molecule 2 is a protein called GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1356	878	226	246	6			
2	E	168	Total	C	N	O	S	0	0	0
			1382	898	229	249	6			

- Molecule 3 is a protein called GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	176	Total	C	N	O	S	0	0	0
			1496	976	241	271	8			
3	F	176	Total	C	N	O	S	0	0	0
			1496	976	242	270	8			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

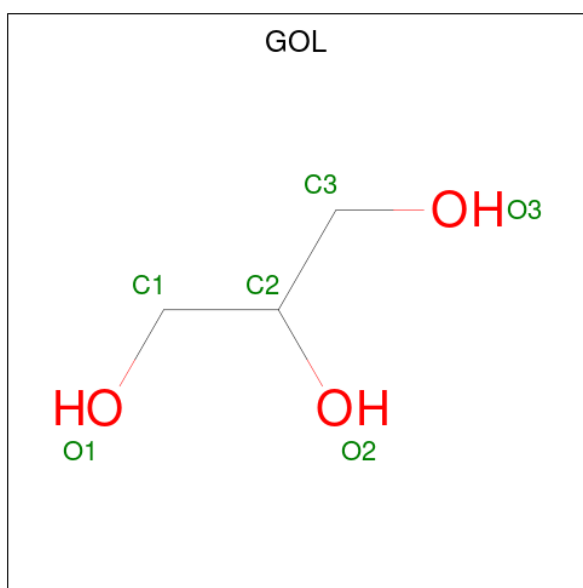
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



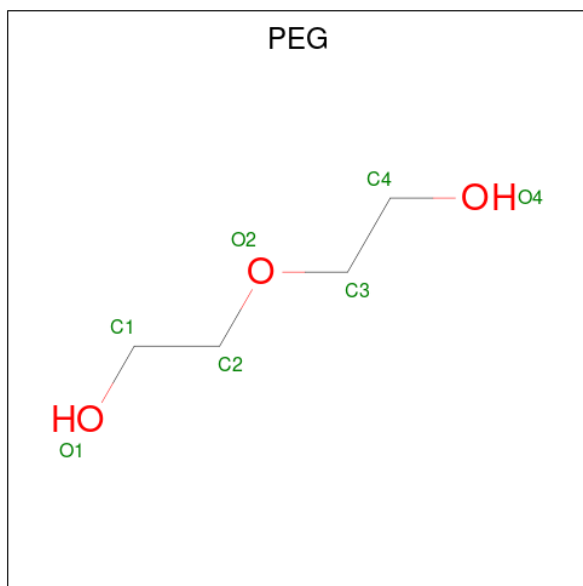
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		
7	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	3	Total	O	0	0
			3	3		
8	D	1	Total	O	0	0
			1	1		
8	E	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.45Å 109.17Å 133.62Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	48.90 – 2.80 48.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.90-2.80) 98.5 (48.90-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.181 , 0.226 0.186 , 0.227	Depositor DCC
R_{free} test set	3895 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14028	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, ACT, GOL, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	0/4238	0.86	4/5757 (0.1%)
1	D	0.49	0/4212	0.82	6/5719 (0.1%)
2	B	0.58	0/1394	0.86	0/1891
2	E	0.57	0/1421	0.88	3/1927 (0.2%)
3	C	0.54	0/1545	0.82	0/2093
3	F	0.50	0/1545	0.77	0/2092
All	All	0.54	0/14355	0.83	13/19479 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	7	LYS	N-CA-C	10.34	125.20	112.59
1	A	2062	LEU	CA-C-N	6.90	126.42	119.24
1	A	2062	LEU	C-N-CA	6.90	126.42	119.24
1	D	2062	LEU	CA-C-N	6.27	125.76	119.24
1	D	2062	LEU	C-N-CA	6.27	125.76	119.24
1	D	1856	VAL	CA-C-N	5.40	125.34	119.78
1	D	1856	VAL	C-N-CA	5.40	125.34	119.78
1	D	1899	ILE	CA-C-N	5.36	125.30	119.78
1	D	1899	ILE	C-N-CA	5.36	125.30	119.78
2	E	7	LYS	CA-C-N	5.15	130.97	121.70
2	E	7	LYS	C-N-CA	5.15	130.97	121.70
1	A	1746	PHE	CA-C-N	5.13	125.16	119.32
1	A	1746	PHE	C-N-CA	5.13	125.16	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4141	0	4176	47	0
1	D	4116	0	4161	40	0
2	B	1356	0	1309	20	0
2	E	1382	0	1344	18	0
3	C	1496	0	1390	9	0
3	F	1496	0	1389	11	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	4	0	3	1	0
5	D	4	0	3	0	0
6	B	6	0	8	1	0
6	E	6	0	8	2	0
7	C	7	0	9	0	0
7	F	7	0	9	0	0
8	B	3	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
All	All	14028	0	13809	127	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1651:LEU:HD11	1:A:1665:ILE:HD13	1.59	0.84
1:D:1651:LEU:HD11	1:D:1665:ILE:HD13	1.58	0.83
1:D:1814:LEU:HD12	2:E:37:MET:HE2	1.64	0.79
1:D:1651:LEU:O	1:D:1661:ARG:NH1	2.24	0.69
1:D:1875:LEU:HD22	1:D:1997:ILE:HG21	1.73	0.68
1:D:1825:ILE:O	1:D:1993:ARG:NH2	2.27	0.67
2:B:60:TRP:HB2	2:B:63:THR:HG22	1.76	0.66
1:A:1651:LEU:O	1:A:1661:ARG:NH1	2.28	0.65
1:A:1875:LEU:HD22	1:A:1997:ILE:HG21	1.79	0.65
1:D:2007:MET:HE2	1:D:2054:ASN:HD22	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:376:MET:HE3	3:C:381:VAL:HG22	1.79	0.65
1:D:1811:ARG:HG2	2:E:37:MET:HE3	1.77	0.65
1:D:2028:ARG:HE	2:E:8:ALA:HB3	1.64	0.63
2:E:60:TRP:HB2	2:E:63:THR:HG22	1.80	0.62
1:D:2028:ARG:NE	2:E:8:ALA:HB3	2.14	0.62
1:D:1627:PHE:CD1	1:D:1691:PRO:HG3	2.36	0.61
1:D:1589:ASN:OD1	1:D:1589:ASN:N	2.34	0.60
1:A:1568:ARG:HD3	1:A:1614:THR:HG21	1.83	0.60
1:A:1627:PHE:CD1	1:A:1691:PRO:HG3	2.37	0.59
1:A:1590:ASP:O	1:A:1593:THR:HB	2.03	0.59
1:A:1627:PHE:CG	1:A:1691:PRO:HG3	2.39	0.57
2:B:153:MET:HE1	2:B:165:ARG:HH12	1.70	0.56
1:A:1745:ALA:HB1	3:C:365:SER:HB2	1.85	0.56
1:D:1979:GLU:HG3	2:E:7:LYS:HE2	1.88	0.56
1:A:1794:SER:H	1:A:1797:ALA:HB3	1.71	0.56
2:E:126:GLU:OE2	6:E:1192:GOL:O1	2.21	0.56
6:E:1192:GOL:H32	3:F:414:SER:HB2	1.90	0.54
1:D:1647:ILE:HG23	1:D:1668:ILE:HD13	1.91	0.53
1:A:2028:ARG:HG3	2:B:8:ALA:O	2.10	0.52
1:D:2028:ARG:NH1	1:D:2032:LYS:HD3	2.24	0.52
1:A:2048:PHE:O	1:A:2052:ILE:HG13	2.10	0.52
2:B:138:ARG:HH11	2:B:190:ILE:HD12	1.73	0.52
1:D:1712:VAL:HA	1:D:1720:ARG:HE	1.75	0.52
2:B:126:GLU:OE2	6:B:1192:GOL:O1	2.28	0.51
1:D:1840:PHE:HE1	1:D:2032:LYS:HD2	1.76	0.51
2:B:50:HIS:CD2	3:C:462:ARG:HD2	2.46	0.51
1:A:1739:HIS:ND1	1:A:1784:ASP:OD2	2.38	0.51
1:A:1857:PRO:HG2	1:A:1869:ILE:HD13	1.92	0.51
2:E:6:LEU:C	2:E:8:ALA:HB2	2.36	0.51
1:A:1867:GLU:HG2	1:A:2000:TYR:OH	2.12	0.50
1:A:1656:PHE:HB3	1:A:1660:THR:HG23	1.93	0.50
1:A:1840:PHE:CE1	1:A:2032:LYS:HD2	2.47	0.50
1:A:1944:ILE:O	1:A:1948:ILE:HG13	2.12	0.50
1:A:2031:LEU:HD12	2:B:9:LEU:HD11	1.94	0.50
2:E:6:LEU:O	2:E:8:ALA:HB2	2.12	0.50
1:D:1617:LYS:HD2	3:F:355:PHE:CE1	2.47	0.49
1:A:2074:ILE:O	1:A:2078:LEU:HG	2.12	0.49
1:A:1779:MET:O	1:A:1783:ILE:HG12	2.10	0.49
1:A:2048:PHE:CE2	1:A:2052:ILE:HD11	2.48	0.49
1:D:1840:PHE:CE1	1:D:2032:LYS:HD2	2.46	0.49
3:F:411:HIS:CG	3:F:412:PRO:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:TRP:HB2	2:B:63:THR:CG2	2.42	0.48
2:B:115:LEU:HD21	3:C:479:PHE:CE2	2.48	0.48
2:E:50:HIS:ND1	3:F:462:ARG:HD2	2.28	0.48
1:D:2007:MET:HE3	1:D:2011:LYS:HD2	1.96	0.48
1:A:2071:ILE:HA	1:A:2074:ILE:HG13	1.96	0.48
2:E:84:VAL:HB	2:E:92:PRO:HG3	1.96	0.47
2:E:115:LEU:HD21	3:F:479:PHE:CE2	2.49	0.47
1:A:2019:LYS:HE3	1:A:2023:GLN:NE2	2.30	0.47
3:C:376:MET:HG3	3:C:380:MET:SD	2.55	0.47
1:D:1597:ILE:O	1:D:1601:VAL:HG23	2.14	0.47
1:D:1641:ASP:OD1	1:D:1698:ASN:ND2	2.45	0.47
2:B:133:ARG:HH22	2:B:138:ARG:HH21	1.62	0.46
1:D:1867:GLU:HG2	1:D:2000:TYR:OH	2.15	0.46
1:D:1779:MET:O	1:D:1783:ILE:HG12	2.15	0.46
1:D:1739:HIS:ND1	1:D:1784:ASP:OD2	2.44	0.46
1:D:1909:LEU:HD11	1:D:1971:ASN:HB3	1.98	0.46
2:B:8:ALA:HB3	2:B:10:VAL:HG22	1.98	0.46
2:B:149:LYS:NZ	2:B:154:GLU:OE1	2.47	0.45
1:A:1601:VAL:HG21	1:A:1654:GLN:CD	2.41	0.45
1:A:1836:PRO:HA	1:A:1837:PRO:HD3	1.79	0.45
1:A:2028:ARG:NH2	2:B:6:LEU:O	2.49	0.45
1:D:1891:LYS:HD3	1:D:1891:LYS:HA	1.61	0.45
1:D:1836:PRO:HA	1:D:1837:PRO:HD3	1.81	0.44
1:D:2019:LYS:HE3	1:D:2023:GLN:NE2	2.32	0.44
2:B:169:VAL:CG1	2:B:178:LYS:HB3	2.47	0.44
1:A:1840:PHE:HE1	1:A:2032:LYS:HD2	1.83	0.44
1:A:1710:ASN:OD1	5:A:3081:ACT:H3	2.16	0.44
1:A:1605:VAL:HG12	1:A:1606:ILE:HG23	2.00	0.44
1:A:1794:SER:N	1:A:1797:ALA:HB3	2.33	0.44
1:A:2059:LEU:HD23	1:A:2059:LEU:HA	1.76	0.44
1:A:1825:ILE:O	1:A:1993:ARG:NH2	2.50	0.43
2:E:169:VAL:CG1	2:E:178:LYS:HB3	2.48	0.43
3:F:465:LEU:HD23	3:F:465:LEU:HA	1.83	0.43
2:E:50:HIS:CE1	3:F:462:ARG:HD2	2.53	0.43
1:A:1865:ASN:OD1	1:A:1867:GLU:HB2	2.18	0.43
1:D:1605:VAL:HG13	1:D:1606:ILE:HG23	2.00	0.43
1:D:2020:LEU:HD23	1:D:2063:PRO:HG2	2.00	0.43
2:E:164:GLU:HB3	2:E:187:TYR:OH	2.18	0.43
1:A:1909:LEU:HD23	1:A:1909:LEU:HA	1.90	0.43
3:C:367:ARG:HD3	3:C:367:ARG:HA	1.85	0.43
1:A:1778:LEU:HD23	1:A:1778:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:463:THR:O	3:C:467:ARG:HG3	2.19	0.43
1:D:1865:ASN:OD1	1:D:1867:GLU:HB2	2.19	0.43
1:A:2057:ILE:H	1:A:2057:ILE:HG13	1.78	0.43
1:D:1665:ILE:HD12	1:D:1665:ILE:HA	1.88	0.43
1:D:1949:GLU:OE2	1:D:1952:ARG:NH1	2.52	0.43
1:A:1871:ALA:O	1:A:1996:ASN:HA	2.19	0.42
2:B:150:ASP:HA	2:B:151:PRO:HD3	1.86	0.42
1:D:1627:PHE:CG	1:D:1691:PRO:HG3	2.54	0.42
3:F:420:GLU:HG3	3:F:421:PRO:HD2	2.02	0.42
2:B:115:LEU:HB2	2:B:128:THR:HG21	2.02	0.42
1:A:2062:LEU:HA	1:A:2063:PRO:HD2	1.77	0.42
1:D:1637:PHE:CG	1:D:1694:ARG:HG2	2.54	0.42
1:A:1601:VAL:HG21	1:A:1654:GLN:OE1	2.20	0.41
1:A:1605:VAL:HG23	3:F:412:PRO:HD3	2.02	0.41
1:A:2031:LEU:HD23	1:A:2031:LEU:HA	1.83	0.41
2:B:84:VAL:HB	2:B:92:PRO:HG3	2.02	0.41
2:E:172:ASP:HA	2:E:173:PRO:HD3	1.79	0.41
3:C:515:LYS:HB2	3:C:532:TRP:CD2	2.56	0.41
1:A:1706:ILE:HD12	1:A:1706:ILE:HA	1.90	0.41
2:B:164:GLU:HB3	2:B:187:TYR:OH	2.20	0.41
1:A:1766:MET:HE2	1:A:1766:MET:HB3	1.80	0.41
1:D:1688:ASN:O	1:D:1691:PRO:HD2	2.20	0.41
2:E:9:LEU:C	2:E:11:PRO:HD3	2.45	0.41
3:F:463:THR:O	3:F:467:ARG:HG3	2.21	0.41
1:D:1701:TYR:HA	1:D:1761:MET:SD	2.61	0.41
3:F:488:TYR:CZ	3:F:492:LEU:HD11	2.55	0.41
1:A:1617:LYS:HD2	3:C:355:PHE:CE1	2.56	0.41
1:A:1738:LEU:HD12	1:A:1738:LEU:HA	1.86	0.41
1:A:1810:LEU:HD21	2:B:34:LEU:HD21	2.02	0.41
1:D:1766:MET:HE2	1:D:1766:MET:HB3	1.87	0.41
1:D:1978:ILE:HD11	1:D:2021:GLU:OE1	2.21	0.41
2:E:9:LEU:HA	2:E:9:LEU:HD12	1.82	0.40
1:A:1982:TYR:HE1	1:A:2028:ARG:HE	1.69	0.40
2:B:132:LEU:HD23	2:B:132:LEU:HA	1.91	0.40
1:D:1641:ASP:HA	1:D:1698:ASN:HD22	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	500/553 (90%)	489 (98%)	11 (2%)	0	100	100
1	D	494/553 (89%)	483 (98%)	11 (2%)	0	100	100
2	B	160/191 (84%)	154 (96%)	5 (3%)	1 (1%)	21	51
2	E	162/191 (85%)	157 (97%)	4 (2%)	1 (1%)	21	51
3	C	170/262 (65%)	162 (95%)	8 (5%)	0	100	100
3	F	170/262 (65%)	164 (96%)	6 (4%)	0	100	100
All	All	1656/2012 (82%)	1609 (97%)	45 (3%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	9	LEU
2	B	9	LEU

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	466/522 (89%)	450 (97%)	16 (3%)	32	68
1	D	465/522 (89%)	456 (98%)	9 (2%)	50	81
2	B	148/177 (84%)	143 (97%)	5 (3%)	32	68
2	E	152/177 (86%)	145 (95%)	7 (5%)	24	58
3	C	161/248 (65%)	158 (98%)	3 (2%)	50	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	160/248 (64%)	156 (98%)	4 (2%)	42 76
All	All	1552/1894 (82%)	1508 (97%)	44 (3%)	38 73

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1569	THR
1	A	1588	ASN
1	A	1593	THR
1	A	1605	VAL
1	A	1741	LEU
1	A	1798	VAL
1	A	1875	LEU
1	A	1923	VAL
1	A	1951	LYS
1	A	1952	ARG
1	A	2028	ARG
1	A	2041	THR
1	A	2052	ILE
1	A	2057	ILE
1	A	2061	ASP
1	A	2071	ILE
2	B	43	ILE
2	B	55	THR
2	B	110	GLU
2	B	138	ARG
2	B	180	GLN
3	C	385	GLU
3	C	516	GLU
3	C	544	ARG
1	D	1585	ARG
1	D	1588	ASN
1	D	1589	ASN
1	D	1795	LYS
1	D	1852	LYS
1	D	1875	LEU
1	D	1923	VAL
1	D	1961	THR
1	D	2008	ASN
2	E	12	LEU
2	E	13	LEU
2	E	43	ILE

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Mol	Chain	Res	Type
2	E	55	THR
2	E	138	ARG
2	E	156	ILE
2	E	180	GLN
3	F	382	SER
3	F	425	VAL
3	F	516	GLU
3	F	544	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1887	HIS
1	A	1975	ASN
1	A	2023	GLN
2	B	50	HIS
1	D	1710	ASN
1	D	1975	ASN
1	D	1991	GLN
1	D	2008	ASN
1	D	2023	GLN
1	D	2054	ASN
2	E	50	HIS
2	E	180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	E	1192	-	5,5,5	0.37	0	5,5,5	0.68	0
7	PEG	F	1561	-	6,6,6	0.68	0	5,5,5	0.66	0
5	ACT	A	3081	-	3,3,3	0.95	0	3,3,3	0.82	0
5	ACT	D	3080	-	3,3,3	0.72	0	3,3,3	1.65	1 (33%)
6	GOL	B	1192	-	5,5,5	0.39	0	5,5,5	0.49	0
7	PEG	C	1561	-	6,6,6	0.65	0	5,5,5	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	F	1561	-	-	1/4/4/4	-
6	GOL	E	1192	-	-	2/4/4/4	-
7	PEG	C	1561	-	-	0/4/4/4	-
6	GOL	B	1192	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3080	ACT	OXT-C-CH3	2.18	124.19	115.05

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1192	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	E	1192	GOL	C1-C2-C3-O3
6	B	1192	GOL	O2-C2-C3-O3
7	F	1561	PEG	O2-C3-C4-O4
6	B	1192	GOL	O1-C1-C2-C3
6	E	1192	GOL	O2-C2-C3-O3
6	B	1192	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1192	GOL	2	0
5	A	3081	ACT	1	0
6	B	1192	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	508/553 (91%)	-0.21	16 (3%)	51	41	37, 57, 115, 174	0
1	D	504/553 (91%)	0.15	20 (3%)	42	33	44, 74, 121, 163	0
2	B	166/191 (86%)	-0.19	7 (4%)	40	32	35, 52, 98, 110	0
2	E	168/191 (87%)	-0.12	10 (5%)	27	21	33, 55, 107, 136	0
3	C	176/262 (67%)	-0.10	10 (5%)	29	22	36, 57, 117, 164	0
3	F	176/262 (67%)	0.03	10 (5%)	29	22	36, 63, 130, 162	0
All	All	1698/2012 (84%)	-0.06	73 (4%)	40	31	33, 62, 118, 174	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1956	ASN	7.7
1	A	1956	ASN	7.0
1	A	1798	VAL	6.7
1	D	1953	THR	6.7
2	B	30	LEU	6.6
2	E	30	LEU	5.6
3	C	346	THR	5.5
1	A	1567	THR	5.3
1	A	2079	VAL	5.2
1	D	1798	VAL	5.1
2	B	13	LEU	5.1
1	A	1953	THR	5.0
3	F	454	LYS	4.7
2	B	5	GLY	4.3
3	F	346	THR	4.3
2	E	48	GLN	4.2
3	C	530	GLU	4.2
2	B	12	LEU	4.1
3	C	372	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	1796	HIS	3.9
2	E	12	LEU	3.8
3	C	373	LEU	3.8
1	A	1657	LYS	3.7
3	F	530	GLU	3.7
2	E	43	ILE	3.6
3	F	372	PRO	3.5
1	D	2078	LEU	3.5
2	E	11	PRO	3.3
2	E	10	VAL	3.3
2	B	11	PRO	3.3
1	D	1797	ALA	3.3
1	A	1569	THR	3.2
2	E	6	LEU	3.2
1	D	1794	SER	3.1
3	C	374	GLN	3.1
3	F	373	LEU	3.1
1	D	1957	ALA	3.1
2	E	13	LEU	3.0
3	C	426	TYR	3.0
1	A	2068	VAL	2.9
2	B	31	GLY	2.9
1	A	2056	ASP	2.9
1	A	1794	SER	2.8
3	C	454	LYS	2.8
3	F	426	TYR	2.8
2	E	5	GLY	2.8
1	D	1657	LYS	2.7
1	A	1796	HIS	2.7
1	D	1567	THR	2.7
1	A	1797	ALA	2.7
3	F	370	MET	2.7
3	F	348	ALA	2.6
2	B	10	VAL	2.6
1	D	2055	ASN	2.6
1	A	1861	ASP	2.6
3	C	370	MET	2.5
1	D	1568	ARG	2.5
1	A	1716	ASP	2.4
3	C	427	PRO	2.4
1	D	2070	GLU	2.3
1	A	2035	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	1632	PRO	2.3
1	D	1716	ASP	2.3
1	D	1795	LYS	2.3
1	D	1853	ASN	2.3
1	D	2061	ASP	2.2
2	E	42	GLY	2.2
1	D	1830	GLU	2.2
3	F	347	ASN	2.2
3	C	455	LYS	2.1
1	D	1604	GLY	2.1
1	A	1570	GLU	2.1
3	F	516	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	D	3080	4/4	0.79	0.26	75,78,88,101	0
5	ACT	A	3081	4/4	0.87	0.20	54,73,78,79	0
7	PEG	C	1561	7/7	0.90	0.24	33,52,74,79	0
7	PEG	F	1561	7/7	0.92	0.19	37,48,57,64	0
6	GOL	E	1192	6/6	0.94	0.09	60,63,65,74	0
6	GOL	B	1192	6/6	0.95	0.10	50,53,58,63	0
4	CA	D	3079	1/1	0.97	0.04	61,61,61,61	0
4	CA	A	3080	1/1	0.98	0.03	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.